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Quantifying Uncertainties of Nucleation and Crystal Growth Model on PAT System Performance for Crystallization Processes

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The introduction of the Process Analytical Technology (PAT) guidance has resulted in increased use of process control applications and process/product quality monitoring in general. This trend is also noticeable for crystallization processes, boosted also by the fact that high quality crystalline products can be produced. During the past years, a unique model-based methodology for PAT system design has been developed [1]. However, it is assumed during the PAT system design that the exact value of the parameters, for example, in the nucleation and crystal growth rate are known. Usually these parameters are usually estimated from experimental data with measurement errors and thus, imply a certain error on the estimated parameters. Consequencely, there is presence of the uncertainties around the value of nucleation and crystal growth model parameter that needs to be taken into account. Therefore the impact and influence of uncertainty in these model parameters on the predicted system performance such as the crystal size distribution (CSD) needs to be quantified and how it affects the system performance from not achieving the target specifications of crystal product needs to be analyzed.

In this work, the ICAS-PAT software [1] has been extended for design of a crystallization process monitoring and control. ICAS-PAT consists of a model library and a knowledge base that allows the user to design/validate PAT systems through a systematic computer aided framework. The objective of this work is to quantify the impact of parameter uncertainty on nucleation and crystal growth models representing crystallization processes [2] for the PAT system design. In order to take into account the uncertainty around the nominal value of each model parameter, the PAT system design is combined with uncertainty and sensitivity analyses. Here the uncertainty analysis using Monte-Carlo simulations is carried out to test the effect of uncertainty of parameters from nucleation and crystal growth kinetic models on the predicted system performance and subsequently to identify the most significant parameters through sensitivity analysis using Standardized Regression Coefficient (SRC) and Morris sampling methods. The application of the uncertainty and sensitivity analyses will be illustrated using the one- and two-dimensional potassium dihydrogen phosphate (KDP) crystallization case study, where the analysis is first carried out under the open loop and followed by the closed loop operation. Through analysis, it is shown that the uncertainty is minimized and the target specifications of crystal products achieved.

Reference:

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